ChE 344 **MIDTERM 2 (IN CLASS PORTION)** Name:_____

Tuesday, March 22nd, 2016

9:30-11:30 AM

Closed book, closed notes. You may use a calculator and the provided equation sheet.

A TAKE-HOME EXAM PROBLEM WILL BE POSTED ON CTOOLS. THE PROBLEM MUST BE TURNED IN ON CTOOLS BY MIDNIGHT ON THE DAY OF THE EXAM. YOU WILL HAVE ONLY **1 HOUR** TO COMPLETE THE PROBLEM AND SUBMIT VIA CTOOLS. LATE SUBMISSIONS WILL ONLY BE PERMITTED IN EXTRAORDINARY CIRCUMSTANCES. THE TAKE HOME PROBLEM WILL BE OPEN-BOOK, OPEN-NOTES, CLOSED INTERNET SEARCH.

Please sign the honor pledge (if applicable):

"I have neither given nor received aid on this exam, nor have I concealed any violation of the honor code."

_____

SCORE:

1. (8 points) _____

2. (12 points) _____

3. (15 points) _____

4. (20 points) _____

5. (25 points) _____

6. (20 points) _____ Take-Home (posted to ctools)

TOTAL (100 points) _____

Problem 1 **(8 Points)**

(Reactor Selection and operating conditions): Using the following sets of reactions, describe the reactor system and conditions that maximizes the selectivity to D. Rates are in (mol/dm^3·s) and concentrations are in (mol/dm^3).

(1) $A + B \rightarrow D$ and $-r_{1A} = 800\exp(-8000K/T)C_A^{0.5}C_B$

(2) $A + B \rightarrow U_1$ and $-r_{2B} = 10\exp(-300K/T)C_AC_B$

(3) $D + B \rightarrow U_2$ and $-r_{3D} = 10^6\exp(-8000K/T)C_DC_B$

Problem 2 **(12 Points)**

(a) A thermal decomposition reaction (A→ B + C) was studied in a differential packed-bed reactor. From the data shown below, determine the reaction rate law parameters.

Experiment	T (K)	Concentration (mol/L)	r(mol/L/s)
1	350	0.5	1.5×10^{-9}
2	350	1.0	4.24×10^{-9}
3	550	0.5	1.21×10^{-3}

Problem 3 **(15 Points)**

The following elementary, liquid phase reactions are carried out isothermally in a CSTR

$A + B \rightarrow C$

$C \rightarrow D$

The initial concentrations of species A and B are 0.05 M and 55.3 M respectively.

Additional information:

$k_1 = 0.007\ dm^3/mol \cdot hr$

$k_2 = 0.2\ hr^{-1}$

(a) Determine expressions for the exit concentrations of relevant species. Clearly state any simplifying assumptions made.

(b) How would you find the value of space time, τ, that maximizes the concentration of species C? DO NOT SOLVE.

Problem 4 **(20 Points)**

Consider a CSTR that is used to carry out a reversible isomerization reaction of the type

$$\boldsymbol{A} \underset{k_r}{\overset{k_f}{\rightleftharpoons}} \boldsymbol{B}$$

Where both the forward and reverse reactions are first order.

Additional Information:

Feed is pure species A

$C_{p,A} = C_{p,B} = 600$ J/mol·K

$k_f = 8.83 \times 10^4 \, e^{(-6290/T)} \, \text{sec}^{-1}$
$k_r = 4.17 \times 10^{15} \, e^{(-14947/T)} \, \text{sec}^{-1}$

Where T is given in degrees Kelvin

(a) Is the reaction exothermic or endothermic? What is the enthalpy of reaction?

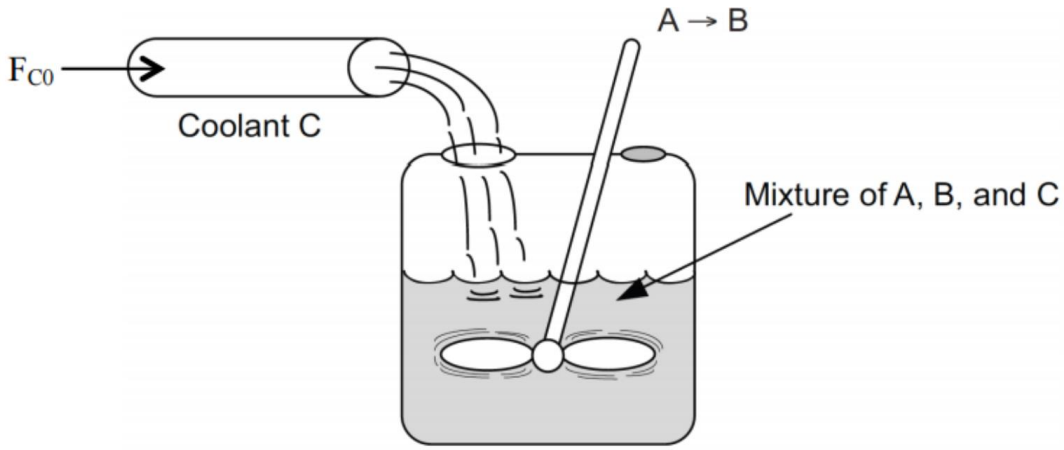
(b) For adiabatic operation, what should the feed temperature be in order to operate at a residence time, τ, of 480 sec and a temperature of 350 K? What is the conversion under these conditions?

(c) Determine the minimum value of τ required to obtain a conversion of 0.5. At what temperature should the reactor operate to achieve these values of X and τ?

Problem 5 **(25 Points)**

A batch reactor is carrying out the irreversible, first-order, liquid-phase, exothermic reaction A→B.

An inert coolant is added to the reaction mixture to control the temperature. The temperature is kept constant by varying the flow rate of the coolant.



(a) Calculate the flow rate of the coolant 2 hr after the start of the reaction. (*Hint: You will need to find an expression for N_A as a function of time*)

(b) What is the remaining number of moles at 2 hr from the start of the reaction and what is the volume change due to addition of the liquid coolant?

Additional Information:

Temperature of reaction: 100 °F
Value of *k* at 100 °F: 1.2 x 10^{-4} s^{-1}
Temperature of coolant: 80 °F
Heat capacity of all components: 0.5 Btu/lb-mol·°F
Density of all components: 50 lb-mol/ft^3
ΔH^o_{RXN}: -25,000 Btu/lb-mol

Initially:
Vessel contains only A (no B or C present)
C_{A0} : 0.5 lb-mol/ft^3
Initial Volume: 50 ft^3

Work Continued from _____

Work Continued from _____

Formula Sheet

Fundamental Equation

$$\frac{dN_A}{dt} = F_{A0} - F_A + \int^V r_A dV$$

Design Equations

	Conversion Basis	Molar Basis
Batch	$N_{A0}\frac{dX}{dt} = -r_A V \qquad t_1 = N_{A0}\int_0^X \frac{dX}{-r_A V}$	$\frac{dN_A}{dt} = r_A V \qquad t_1 = \int_{N_{A_1}}^{N_{A_0}} \frac{dN_A}{-r_A V}$
CSTR	$V = \frac{F_{A0}(X_{out} - X_{in})}{-r_{A_{out}}}$	$V = \frac{F_{Ain} - F_{Aout}}{-r_{A_{out}}}$
PFR	$F_{A0}\frac{dX}{dV} = -r_A \qquad V_1 = F_{A0}\int_{X_{in}}^{X_{out}} \frac{dX}{-r_A}$	$\frac{dF_A}{dV} = r_A \qquad V_1 = \int_{F_{A_1}}^{F_{A_0}} \frac{dF_A}{-r_A}$
PBR	$F_{A0}\frac{dX}{dW} = -r'_A \qquad W_1 = F_{A0}\int_{X_{in}}^{X_{out}} \frac{dX}{-r'_A}$	$\frac{dF_A}{dW} = r'_A \qquad W_1 = \int_{F_{A_1}}^{F_{A_0}} \frac{dF_A}{-r'_A}$

Ideal gas law: $pV = nRT \qquad R = 8.314\frac{J}{mol.K} = 1.987\frac{cal}{mol.K}$

Arrhenius Equation: $k_A(T) = A \cdot \exp\left[\frac{E_A}{-RT}\right] \qquad k_A(T) = k_A(T_0) \cdot \exp\left[\frac{E_A}{R}\left(\frac{1}{T_0} - \frac{1}{T}\right)\right]$

$$K_C(T) = K_C(T_0) \cdot \exp\left[\frac{\Delta H^o_{rxn}}{R}\left(\frac{1}{T_0} - \frac{1}{T}\right)\right]$$

Stoichiometry:

For Reaction: $aA + bB \rightarrow cC + dD$ Liquid Phase: $C_i = C_{A0}(\Theta_i - v_i X)$

Gas Phase: $C_i = \frac{C_{A0}(\Theta_i + v_i X)}{1+\varepsilon X}\left(\frac{P}{P_0}\right)\left(\frac{T_0}{T}\right) \qquad v = v_0(1+\varepsilon X)\left(\frac{T}{T_0}\right)\left(\frac{P_0}{P}\right)$

$$\Theta_i = \frac{F_{i0}}{F_{A0}} = \frac{C_{i0}}{C_{A0}} = \frac{y_{i0}}{y_{A0}} \qquad \delta = \frac{d}{a} + \frac{c}{a} - \frac{b}{a} - 1 \qquad \varepsilon = y_{A0}\delta$$

Packed Beds: laminar turbulent

$$\frac{dP}{dz} = -\frac{G}{\rho g_c D_P}\left(\frac{1-\phi}{\phi^3}\right)\left[\frac{150(1-\phi)\mu}{D_P} + 1.75G\right] \qquad \frac{dP}{dW} = -\frac{\alpha}{2}\frac{P_0}{P/P_0}\left(\frac{T}{T_0}\right)(1 + y_{A0}\delta X)$$

$$\beta_0 = -\frac{G}{\rho_0 g_c D_P}\left(\frac{1-\phi}{\phi^3}\right)\left[\frac{150(1-\phi)\mu}{D_P} + 1.75G\right] \qquad \alpha = \frac{2\beta_0}{A_C\rho_c(1-\phi)P_0} \qquad dW = (1-\phi)A_C\rho_c\, dz$$

If isothermal and $\delta = 0$ or X is very small: $\frac{P}{P_0} = (1-\alpha W)^{1/2} = \left(1 - \frac{2\gamma W}{P_0}\right)^{1/2}$

Energy Balance

$$\frac{d\hat{E}_{sys}}{dt} = \dot{Q} - \dot{W}_s + \sum F_i H_i\Big|_{in} - \sum F_i H_i\Big|_{out}$$

For Steady State System in Single Phase
$0 = \dot{Q} - \dot{W}_s - F_{A0}\sum_{i=1}^{n} \Theta_i \overline{C_{P_i}}(T - T_{i0}) - \Delta H_{Rx}(T) F_{A0} X$ where $H_{Rx}(T) = \Delta H^o_{Rx}(T_R) + \underbrace{\Delta C_p}_{\Sigma \nu_i C_{Pi}}(T - T_R)$

Adiabatic System (CSTR, PFR, PBR, Batch)
Conversion $X = \frac{\Sigma \Theta_i C_{P_i}(T - T_0)}{-[\Delta H^{\circ}_{Rx}(T_R) + \Delta C_P(T - T_R)]}$
Temperature $T = \frac{X[-\Delta H^{\circ}_{Rx}(T_R)] + \Sigma \Theta_i C_{P_i} T_0 + X \Delta C_P T_R}{\Sigma \Theta_i C_{P_i} + X \Delta C_P}$

PFR with heat exchange

$$\frac{dT}{dV} = \frac{\overbrace{r_A \Delta H_{Rx}}^{\substack{Q_g \\ Heat\ "Generated"}} - \overbrace{Ua(T - T_a)}^{\substack{Q_r \\ Heat\ "Removed"}}}{\Sigma F_i C_{P_i}}$$

Unsteady State CSTR and Semibatch

$$\frac{dT}{dt} = \frac{\dot{Q} - \dot{W}_s - \sum F_{i0}\overline{C_{P_i}}(T - T_0) + (-\Delta H_{Rx})(-r_A V)}{\Sigma N_i C_{P_i}}$$

Multiple Reactions:

Selectivity and Yield

Instantaneous Selectivity	$S_{D/U} = {r_D}/{r_U}$
Overall Selectivity	$\tilde{S}_{D/U} = {F_D}/{F_U}$
Instantaneous Yield	$Y_{D/A} = {r_D}/{-r_A}$
Overall Yield	$\tilde{Y}_{D/U} = {F_D}/{F_{A0} - F_A}$

Integrals:

$$\int_0^X x^a dx = \frac{x^{a+1}}{a+1}, \qquad a \neq -1$$

$$\int_0^X x^{-1} dx = \ln(x)$$

$$\int_0^X \frac{dX}{1-X} = \ln\left(\frac{1}{1-X}\right)$$

$$\int_0^X \frac{dX}{(1-X)^2} = \frac{X}{1-X}$$

$$\int_0^X \frac{dX}{1+\varepsilon X} = \frac{1}{\varepsilon}\ln(1+\varepsilon X)$$

$$\int_0^X \frac{1+\varepsilon X}{1-X} dX = (1+\varepsilon)\ln\left(\frac{1}{1-X}\right) - \varepsilon X$$

$$\int_0^X \frac{1+\varepsilon X}{(1-X)^2} dX = \frac{(1+\varepsilon)\mathrm{X}}{1-X} - \varepsilon\ln\left(\frac{1}{1-X}\right)$$

$$\int_0^W (1-\alpha W)^{1/2} dW = \frac{2}{3\alpha}\left[1 - (1-\alpha W)^{3/2}\right]$$

$$\int_0^X \frac{(1+\varepsilon X)^2}{(1-X)^2}\,dX = 2\varepsilon(1+\varepsilon)\ln(1-X) + \varepsilon^2 X + \frac{(1+\varepsilon)^2 X}{1-X}$$

$$\int_0^X \frac{dX}{(1-X)(\Theta_B - X)} = \frac{1}{\Theta_B - 1}\ln\left(\frac{\Theta_B - X}{\Theta_B(1-X)}\right), \qquad \Theta_B \neq 1$$

$$\frac{dy}{dt} + P(t)y = Q(t), \qquad I(t) = e^{\int P(t)}, \qquad \frac{d\big(yI(t)\big)}{dt} = Q(t)I(t),$$

$$y = \frac{1}{I(t)}\int Q(t)I(t)dt$$

Roots for: $ax^2 + bx + c$ $\qquad \dfrac{-b \pm \sqrt{b^2-4ac}}{2a}$